DETERMINATION OF TEMPERATURE, VELOCITY, AND CONCENTRATION PROFILES

IN THE MIXING LAYER BETWEEN A ROCKET EXHAUST JET AND

THE SURROUNDING SUPERSONIC AIR STREAM

III. PROCEDURE FOR COMPUTATIONS AND

PRELIMINARY RESULTS FOR A TYPICAL CASE

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23 March 1960

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34

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CONTENTS

ILLUSTRATIONS

DETERMINATION OF TEMPERATURE, VELOCITY, AND CONCENTRATION PROFILES IN THE MIXING LAYER BETWEEN A ROCKET EXHAUST JET AND THE SURROUNDING SUPERSONIC AIR STREAM

PART III. PROCEDURE FOR COMPUTATIONS AND PRELIMINARY RESULTS FOR A TYPICAL CASE

J. Vasiliu

ABSTRACT

In Section I of this Part, the method of obtaining the
initial and boundary conditions for available inviscid jet
flow solutions is discussed. Simple relations for the determi-
nation of the temperatures, velocities, Mach numbers, pres-
sures, and pressure gradients are derived. In Section II the
thermodynamic functions required in the calculations are dis-
cussed in detail and listed in Table I. A program written in
Fortran II that makes it possible to carry out the solution
of the problem on an IBM-704 computer is described briefly.
Finally one typical case is considered and plots of velocity,
temperature, and concentration profiles are given for the
initial stages of development of the mixing layer.

I. DETERMINATION OF THE BOUNDARY CONDITIONS

It was pointed out in Section IV of Part II that values of the
velocities and temperatures at the upper and lower boundaries may be
obtained from the inviscid flow solution of the jet. Such a solution
was obtained[1] by the method of characteristics for the case of an
axially symmetric jet of gas, with constant ratio of specific heats,
issuing into a supersonic air stream. For lack of other data, the results
of this analysis will be used to obtain the boundary conditions for the
two-dimensional mixing layer considered here.

A. Initial Conditions

The conditions at $x = 0$ require a knowledge of the velocity and
temperature of the jet and the air stream at a section normal to the

1

boundary. The flow parameters available from the inviscid flow solution[1] are indicated in Figure 1. It is noted that the Mach number of the jet at a section normal to the boundary, denoted by M_e, is different from the Mach number at a section normal to the exit, denoted by M_{jet}, the former being larger in view of the expansion taking place at the periphery of the nozzle. The initial conditions will be based on M_e. Using the total temperature of the jet, T_{T_j}, and the constant ratio of specific heats, γ_{jt}, one has

$$T_e = \frac{T_{T_j}}{1 + \frac{\gamma_{jt}-1}{2} M_e^2} \tag{1}$$

The velocity is expressed in terms of the Mach number and temperature from the relation

$$U_e = M_e \sqrt{\gamma_{jt} g R_{m_e} T_e} \tag{2}$$

Where R_{m_e} is the gas constant for the mixture at the exit conditions given by

$$R_{m_e} = \frac{R}{W_{m_e}} \tag{3}$$

with W_{m_e}, the molecular weight of the mixture at the exit, given by

$$W_{m_e} = \sum_i W_i X_i \ .$$

Substituting Eq. (3) into (2), and using consistent units, one finds

$$U_e = 222.97 \ M_e \ \sqrt{\frac{\gamma_{jt} T_e}{W_{m_e}}} \ (\text{ft/sec}) \tag{4}$$

For the air-stream side one has, from the energy equation, using the total temperature of the stream T_{T_s}

$$\frac{T_{T_s}}{T_\infty} = 1 + \frac{\gamma_s-1}{2} M_\infty^2$$
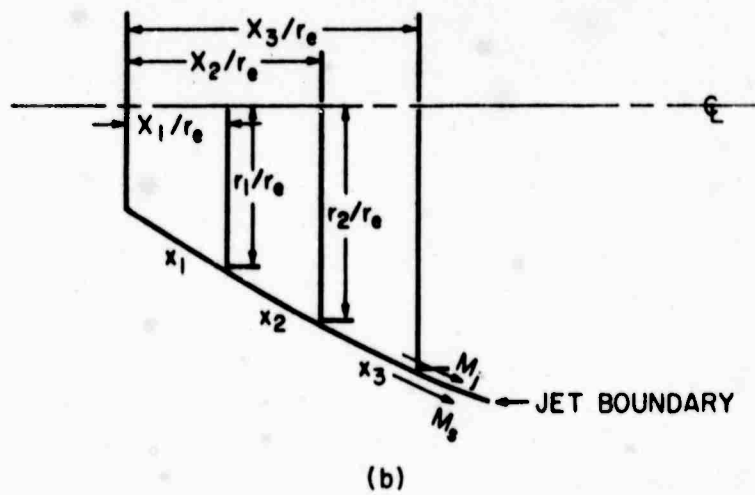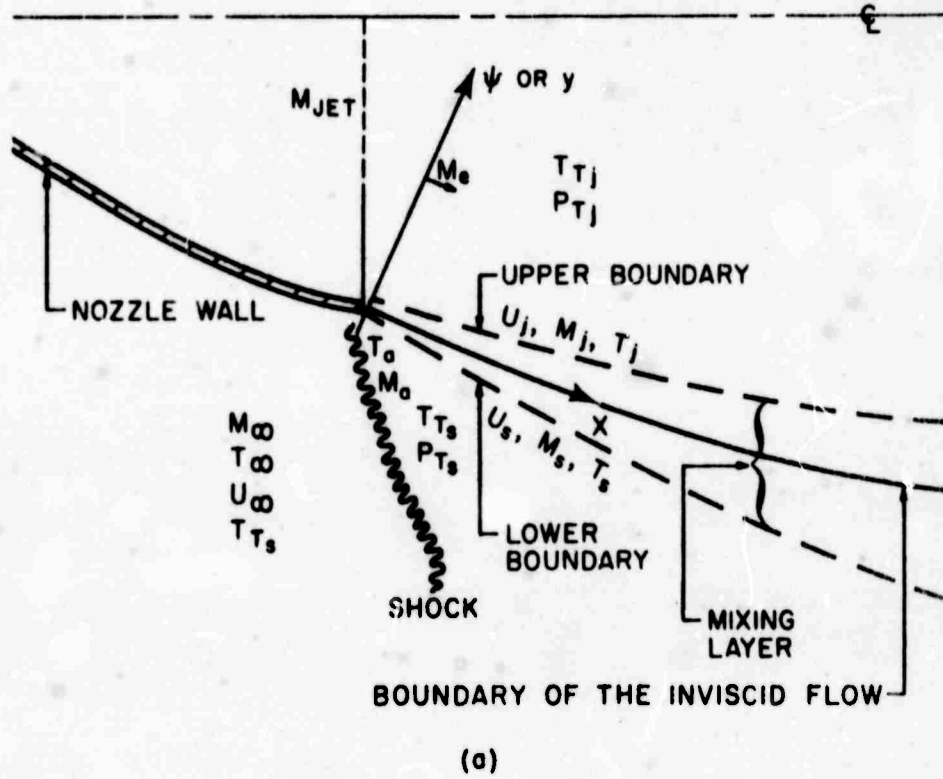
2

(a)

(b)

FIGURE 1   SCHEMATIC DIAGRAM OF THE MIXING LAYER

3

and

$$\frac{T_s}{T_a} = 1 + \frac{\gamma_s - 1}{2} M_a^2$$

so that

$$T_a = T_\infty \left[\frac{1 + \frac{\gamma_s - 1}{2} M_\infty^2}{1 + \frac{\gamma_s - 1}{2} M_a^2} \right] \qquad (5)$$

The velocity can be obtained, as before, from a relation analogous to Eq. (4)

$$U_a = 222.97 \, M_a \sqrt{\frac{\gamma_s T_a}{W_{m_a}}} \, (\text{ft/sec}) \qquad (6)$$

where W_{m_a}, the molecular weight of the air stream, is given by

$$W_{m_a} = \frac{1}{\displaystyle\sum_i \frac{(C_i)_a}{W_i}} \qquad (7)$$

The concentration of species at the nozzle exit can be obtained from an analysis of the problem of chemical reactions during the expansion of premixed gases through the nozzle.[2] It is indicated here that one may consider the chemical reactions in the flow to be in local equilibrium up to a certain point of the expansion, and to be frozen at those values thereafter, up to the nozzle exit area and further downstream. Such a treatment yields values of the specific impulse which are in good agreement with observations on actual nozzles.[2] The three additional species, namely, H, O, and OH, listed by Neu, and Boynton[2], are neglected in this work. The mole fractions of the constituents used in the calculations are given in Section III. For the air stream, the standard argon-free air composition will be used.

B. Boundary Conditions

The method of characteristics[1] gives the Mach number of the flow at either side of the jet boundary in terms of the dimensionless axial

4

distance, X/r_e, and the dimensionless radial distance, r/r_e. It is easily seen from Figure 1.b that the dimensionless coordinate x used in this work can be related to the above coordinates (after linearizing each small segment on the boundary) by means of the relation

$$(x)_i = \sum_i \sqrt{\left[\left(\frac{X}{r_e}\right)_i - \left(\frac{X}{r_e}\right)_{i-1}\right]^2 + \left[\left(\frac{r}{r_e}\right)_i - \left(\frac{r}{r_e}\right)_{i-1}\right]^2} \tag{8}$$

where "i" denotes the points at which the values of M_j and M_s are known (see Table II). For calculations on the computer, the values of M_j and M_s may be listed as a function of $(x)_i$, or these Mach numbers can be expressed as polynomials in x. It has been found that the maximum error incurred in using a 4th degree polynomial approximation does not exceed 0.30 percent. Values of the coefficients for a specific case, are given in the section on input data.

1. Upper Boundary

    In view of the above, the Mach number on the jet side will be given by the relation

$$M_j = \alpha_o + \alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3 + \alpha_4 x^4 \tag{9}$$

The temperature at this boundary can then be expressed in terms of this Mach number as

$$T_j = \frac{T_{T_j}}{1 + \frac{\gamma_{jt}-1}{2} M_j^2} \tag{10}$$

or, in dimensionless form and using the notation of Part II for the grid points at the boundary,

$$T_{N+1,\ell} \equiv T_j^* \equiv \frac{T_j}{T_o} = \frac{T_{T_j}/T_o}{1 + \frac{\gamma_{jt}-1}{2} M_j^2} \tag{11}$$

The velocity is obtained by a relation analogous to Eq. (4), i.e.

$$U_j = 222.97 \, M_j \sqrt{\frac{\gamma_{jt} T_j}{W_{m_e}}} \tag{12}$$

5

which can be rewritten in the following dimensionless form

$$u_{N+1, l} \equiv \frac{U_j}{U_o} = 222.97 \frac{M_j}{U_o} \sqrt{\frac{\gamma_{jt} T_{N+1, l} T_o}{W_{m_e}}} \tag{13}$$

It is noted that in Eq. (12) and (13) the molecular weight of the mixture at the upper boundary is the same as that at the nozzle exit. This is consistent with the remaining boundary condition i.e.

$$c_{N+1, l}^1 = (c^1)_e \tag{14}$$

which is based on the assumption that the composition of the jet, down-stream from the nozzle, remains frozen at the conditions at the exit. Equation (11), (13) and (14) constitute the boundary conditions for the upper boundary of the mixing layer.

2. Lower Boundary

For the air-stream side, the Mach number will be obtained from the relation

$$M_s = \beta_{co} + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4 \tag{15}$$

Based on this Mach number, the temperature at this boundary is given by a relation analogous to Eq. (5)

$$T_s = T_\infty \left[\frac{1 + \frac{\gamma_s - 1}{2} M_\infty^2}{1 + \frac{\gamma_s - 1}{2} M_s^2} \right] \tag{16}$$

or, in dimensionless form, and in terms of the notation for a grid point on the lower boundary,

$$T_{0, l} \equiv \frac{T_s}{T_o} = \frac{T_\infty}{T_o} \left[\frac{1 + \frac{\gamma_s - 1}{2} M_\infty^2}{1 + \frac{\gamma_s - 1}{2} M_s^2} \right] \tag{17}$$

The velocity can be determined, from a relation analogous to Eq. (6):

$$U_s = 222.97 \, M_s \sqrt{\frac{\gamma_s T_s}{W_{m_a}}} \tag{18}$$

6

or,

$$u_{0,l} \equiv \frac{U_s}{U_o} = 222.97 \frac{M_s}{U_o} \sqrt{\frac{\gamma_s T_{o,l} T_o}{W_{m_a}}} \tag{19}$$

where W_{m_a} is given by Eq. (7). The additional condition on the concentrations is

$$c^1_{0,l} = (c^1)_a \tag{20}$$

Equation (17), (19) and (20) constitute the boundary conditions for the lower boundary of the mixing layer.

C. Relations for the Pressure and Pressure Gradient

The inviscid flow solution[1] yields the stagnation pressure at both sides of the boundary. Values of the static pressure, required in this work, can be obtained from this pressure. Since the static pressure must be balanced at the jet boundary, one may use the flow parameters at either side in carrying out the calculations. Selecting, arbitrarily, the stream side stagnation pressure, p_{T_s}, and Mach number, M_s, the static pressure, p_s, is given by

$$p_s = \frac{p_{T_s}}{\left(1 + \frac{\gamma_s - 1}{2} M_s^2\right)^{\gamma_s/(\gamma_s - 1)}} \tag{21}$$

or, in dimensionless form,

$$p \equiv \frac{p_s}{p_o} = \frac{p_{T_s}/p_o}{\left(1 + \frac{\gamma_s - 1}{2} M_s^2\right)^{\gamma_s/(\gamma_s - 1)}} \tag{22}$$

The dimensionless pressure gradient is obtained by differentiating the above expression

$$p_x \equiv \frac{dp}{dx} = - \frac{\gamma_s M_s p}{\left(1 + \frac{\gamma_s - 1}{2} M_s^2\right)} \frac{dM_s}{dx} \tag{23}$$

7

From Eq. (15)

$$\frac{dM_s}{dx} = \beta_1 + 2\beta_2 x + 3\beta_3 x^2 + 4\beta_4 x^3 \tag{24}$$

Substituting Eq. (24) into Eq. (23), the pressure gradient is found to be

$$p_x = - \frac{\gamma_s M_s p}{\left(1 + \frac{\gamma_s - 1}{2} M_s^2\right)}\left(\beta_1 + 2\beta_2 x + 3\beta_3 x^2 + 4\beta_4 x^3\right) \tag{25}$$

This equation is to be calculated at the point $x = \bar{x}$ as required in Part II. The pressure at the nozzle exit can be obtained from the stagnation pressure of the jet. Thus

$$p_e = \frac{p_{T_j}}{\left(1 + \frac{\gamma_{jt} - 1}{2} M_e^2\right)^{\gamma_{jt}/\gamma_{jt} - 1}} \tag{26}$$

II. DATA REQUIRED IN THE CALCULATIONS

A. Thermodynamic Functions

In Part II a function $f_1(T)$, Eq. (36), has been used in the equation for the dimensionless specific heat of each species to denote the temperature dependent molar specific heat of the gas. This function can be expressed by means of approximating polynomials such as those given by Sweigert and Beardsley. The equations are of two general forms, and they are valid within a given range

$$f_1(T) = a - \frac{b}{T} + \frac{c}{T^2}$$

or

$$f_1(T) = a - \frac{b}{\sqrt{T}} + \frac{c}{T}$$

where T is the temperature in °R. The equations corresponding to each species are listed in column 8 of Table I. Their accuracy was checked against the values given in the Gas Tables for the range of 500-5000°R. The maximum error found is 0.50 percent for the CO_2-curve, 0.80 percent

8

for the O_2- and H_2-curve, 1.0 percent for the CO-curve, 1.5 percent for the N_2, and 2.0 percent for the H_2O curve. It is noted that, in Table I, T is the dimensionless temperature.

For temperatures from 500°R down to about 250°R, the specific heat may be assumed constant. Values taken from the Gas Tables are also listed in column 8. For O_2, H_2O, CO, N_2 this assumption leads to negligible error. For H_2 and CO_2 the constant values used were selected arbitrarily so as to give small errors (a maximum of 2.5 percent) above 300°R. Below this temperature, the error for these two gases is appreciable, and it may become necessary to use approximating equations.

The function $f_i'(T)$ tabulated in column 9 is the derivative of $f_i(T)$ with respect to the dimensionless temperature; it appears in some terms of the energy equation.

A method of calculating the dimensionless enthalpy of each species is discussed in Part II. The equation obtained there [Eq. (41)], is

$$ h_i = \frac{1}{W_i c_{po} T_o} \left[h_{B_i} + G_i(T) - 1.8 \Delta h f_i^o \right] $$

Here $G_i(T)$ is the integral of $f_i(T)$, and is given in column 10. Below 500°R this term is set equal to zero as noted in Part II. The constant h_{B_i} was computed from the relation [Eq. (40) of Part II]

$$ h_{B_i} = \int_0^{500} f_i(T) dT - G_i(500) \qquad T > 500°R $$

For temperatures below 500°R h_{B_i} is given by Eq. (42), i.e.

$$ h_{B_i} = f_i(T) T \qquad T < 500°R $$

The above values of h_{B_i} are tabulated in column 7 of Table I. In the case of CO_2, for T < 500°R, the value of $f_i(T)$ used in computing h_{B_i} is different from the one listed in column 8. This selection was made in order to reduce the error in the approximation. Values of the enthalpy obtained by the above procedure were compared with values in the Gas

9

Tables at various temperatures. The error was found to be small----less
than one percent in most of the cases, (exceptions were H_2 at low temper-
atures, where the error is about 2 percent, and CO_2 in the neighborhood
of 500°R, where the error is found to be 4 percent). These errors be-
come negligible, in view of the large values of the heats of reaction.

The equilibrium constant $K_{p_k}(T)$ is discussed in Part II, where the
following equation is given:

$$K_{p_k}(T) = \left\{ 10^{\left[10^{F_k(T)}\right]} \right\}^2$$

The function $F_k(T)$ may be obtained from tabulated values of the
equilibrium constant, K_p, given in terms of pressures (see S.S. Penner,
"Chemistry Problems in Jet Propulsion"). It was found that a good fit
to these values is obtained for both the H_2O- and the CO_2- reactions
when $F_k(T)$ is expressed as a fifth degree polynomial. In the range of
1200-3000°K, the error in the values of $K_{p_k}(T)$ is about 0.1 percent
for the H_2O-reaction, and about 3.0 percent for the CO_2-reaction. The
polynomials are given in column 11 of Table I. The variable, T', shown
there is a function of the dimensionless temperature, T, and is given
by the relation

$$T' = \frac{1}{1800} \left[\frac{TT_0}{1.8} - 1200 \right]$$

The factor 1.80 is used to convert the temperature to degrees Kelvin,
as required. It was pointed out in Part II that, below approximately
1800°R, the equilibrium constant becomes large enough that the ratio
K_c'/K_c may be considered zero. It is unnecessary, therefore, to provide
a curve-fit for temperatures below this limit.

The values of Δhf_1^0, the heats of reaction listed in column 6, were
obtained from NBS Circular 500 (Selected Values of Chemical Thermodynamic
Properties, February 1952), and are given at absolute zero for the
component in the gaseous state. The values of B_1 and E_1, given in column
5 and 6, are somewhat uncertain.* Because of the assumption that

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*These values were suggested by F. Boynton, member of the Applied
Research Group, Convair Astronautics

oxidation of H_2, and CO proceed according to a single step chemical reaction (discussed in Section III-B2 of Part II) it becomes difficult to deduce values of B_i and E_i from the meager experimental data available at the present time. For this reason B_i has been grouped, along with other reference quantities, into a single parameter, K_{B_k}, as shown in the above-mentioned section. The solution of the problem can thus be carried out parametrically for various values of K_{B_k} in the range of variation of B_i.

B.   Reference Values and Dimensionless Parameters

The reference values used in non-dimensionalizing the flow parameters may be expressed arbitrarily in terms of the initial values in the jet and the air stream. One may use the mean values for the velocities and temperatures. Thus,

$$U_o = \frac{U_c + U_a}{2} \tag{27}$$

$$T_o = \frac{T_c + T_a}{2} \tag{28}$$

For a reference pressure, one may use the pressure at the exit of the nozzle:

$$p_o = p_e \quad (lbs/in^2) \tag{29}$$

and, for a reference molecular weight, the molecular weight of the jet mixture at the nozzle exit:

$$W_{m_o} = W_{m_e} = \sum W_i X_i \quad . \tag{30}$$

A reference density is obtained from the equation of state, using the reference values given above. Thus,

$$\rho_o = \frac{p_o}{T_o} \frac{W_{m_o}}{R} \tag{31}$$

In consistent units, this equation is rewritten as

$$\rho_o = \frac{144}{1545.43} \frac{p_o W_{m_o}}{T_o} \quad (lbs/ft^3) \tag{31a}$$

11

The reference specific heat is set equal to the specific heat of the mixture at the nozzle exit. The specific heat of each species at the exit is given by

$$\left(c_{pi}\right)_e = \frac{1}{W_i} \, f_i\left(\frac{T_e}{T_o}\right) \tag{32}$$

and the reference specific heat is then

$$c_{po} = c_{pe} = \sum_i \left(C_i\right)_e \left(c_{pi}\right)_e \tag{33}$$

This equation can be modified somewhat by using the relation

$$\left(C_i\right)_e = \frac{W_i X_i}{\sum_i W_i X_i} = \frac{W_i X_i}{W_{m_o}}$$

Substituting also Eq. (32), Eq. (33) becomes

$$c_{po} = \frac{1}{W_{m_o}} \sum_i X_i \, f_i\left(\frac{T_e}{T_o}\right) \tag{34}$$

where the function $f_i(T_e/T_o)$ can be computed from column 8 of Table I.

The dimensionless parameters which are functions of the reference values given above will be rewritten here in consistent units. These are,

$$K_{p_o} = \frac{p_o}{\rho_o U_o^2} = \frac{R T_o}{W_{m_o} U_o^2}$$

or

$$K_{p_o} = 32.17 \times 1545.43 \, \frac{T_o}{W_{m_o} U_o^2} \tag{35}$$

and

$$\beta_o = \frac{U_o^2}{c_{po} T_o}$$

or, in consistent units,

$$\beta_o = \frac{1}{32.17 \times 778.26} \, \frac{U_o^2}{c_{po} T_o} \tag{36}$$

12

TABLE I. THERMODYNAMIC DATA AND RELATED FUNCTIONS

(The temperature "T" used here is the dimensionless temperature.)

$i \equiv k$	Species	v_i gm/gm-mole lb/lb-mole	γ_i	δ_i $\pi_o < 500$	B_i $(cm^3/mole)^2$ $sec(°K)^{\gamma_i}$	E_i (cal/gm-mole)	Δh_i^o (cal/gm-mole) $\pi_o \geq 500$	Δh_i^o $\pi_o < 500$	h_{B_i} (Btu/lb-mole) $\pi_o \geq 500$	h_{B_i} $\pi_o < 500$	$f_i(T)$ (Btu/lb-mole °R) (cal/gm-mole °K) $\pi_o \geq 500$	$f_i(T)$ $\pi_o < 500$
1	H_2O	18.016	0.50	-1.0	9×10^{10}	1.60×10^4	5.71×10^4	0	-25,889	7.97	$19.86 - \dfrac{227}{\sqrt{\pi_o}} + \dfrac{7500}{\pi_o}$	7.97
2	H_2	2.016	0.50	-1.0	9×10^{10}	1.60×10^4	0	0	-461	6.64	$5.76 + 0.578 \times 10^{-3}\pi_o + \dfrac{20}{\sqrt{\pi_o}}$	6.64
3	O_2	32.00	--	0	0	0	0	0	-4,110	6.96	$11.515 - \dfrac{172}{\sqrt{\pi_o}} + \dfrac{1530}{\pi_o}$	6.96
4	CO_2	44.010	0.50	-1.0	3×10^{11}	2.5×10^4	6.764×10^4	0	39,015	7.10	$16.2 - \dfrac{6.53 \times 10^5}{\pi_o} + \dfrac{1.41 \times 10^8}{(\pi_o)^2}$	3.20
5	CO	28.010	0.50	-1.0	3×10^{11}	2.5×10^4	0	0	23,532	6.95	$9.46 - \dfrac{2.29 \times 10^5}{\pi_o} + \dfrac{1.07 \times 10^8}{(\pi_o)^2}$	5.35
6	N_2	28.016	--	0	0	0	0	0	--	6.95	$9.47 - \dfrac{2.47 \times 10^5}{\pi_o} + \dfrac{1.16 \times 10^8}{(\pi_o)^2}$	6.95

$i \equiv k$	Species	$f_i(T)$ $\pi_o \geq 500$	$f_i(T)$ $\pi_o < 500$	$G_i(T)$ $\pi_o \geq 500$	$G_i(T)$ $\pi_o < 500$	$\gamma_k(T)$
1	H_2O	$\dfrac{298.5}{T\sqrt{\pi_o}} - \dfrac{7500}{T(\pi_o)}$	0	$19.86(\pi_o) - 1194\sqrt{\pi_o} + 7500 \ln(\pi_o)$	0	$b_o + b_1 T' + b_2 T'^2 + b_3 T'^3 + b_4 T'^4 + b_5$
2	H_2	$0.578 \times 10^{-3}\pi_o - \dfrac{10}{T\sqrt{\pi_o}}$	0	$5.76(\pi_o) + 0.289 \times 10^{-3}(\pi_o)^2 + 40\sqrt{\pi_o}$	0	
3	O_2	$\dfrac{86}{T\sqrt{\pi_o}} - \dfrac{1530}{T(\pi_o)}$	0	$11.515(\pi_o) - 344\sqrt{\pi_o} + 1530 \ln(\pi_o)$	0	--
4	CO_2	$\dfrac{6.53 \times 10^5}{T(\pi_o)} - \dfrac{2.82 \times 10^8}{T(\pi_o)^2}$	0	$16.20(\pi_o) - 6.53 \times 10^5 \ln(\pi_o) - \dfrac{1.41 \times 10^8}{(\pi_o)}$	0	$a_o + a_1 T' + a_2 T'^2 + a_3 T'^3 + a_4 T'^4 + a_5 T'^5$
5	CO	$\dfrac{2.29 \times 10^5}{T(\pi_o)} - \dfrac{2.14 \times 10^8}{T(\pi_o)^2}$	0	$3.46(\pi_o) - 3.29 \times 10^5 \ln(\pi_o) - \dfrac{1.07 \times 10^8}{(\pi_o)}$	0	
6	N_2	$\dfrac{2.47 \times 10^5}{T(\pi_o)} - \dfrac{2.32 \times 10^8}{T(\pi_o)^2}$	0	--	--	--

Coefficients for $\gamma_k(T)$

$a_o = .8877$
$a_1 = -.9533$
$a_2 = -.2969$
$a_3 = 1.445$
$a_4 = -2.070$
$a_5 = .6697$
$b_o = .5774$
$b_1 = -.8946$
$b_2 = .3968$
$b_3 = -.4501$
$b_4 = .2858$
$b_5 = -.1139$

Two other dimensionless parameters, appearing in the expression for the
rate of production of species, may also be included in this list. The
dimensionless frequency factor is given by [see Part II, Eq. (24)]

$$K_{B_k} = \frac{2LB_k \rho_o^2 (T_o)^{\gamma_k}}{U_o \left(W_{m_o}\right)^2}$$

or, in consistent units, expressing B_k in $(cm^3)^2/(mole)^2/(°K)^{\gamma_k}/sec$, and
ρ_o in lbs/ft^3, as given by Eq. (31a),

$$K_{B_k} = 5.1528 \times 10^{-4} \frac{\rho_o^2}{\left(W_{m_o}\right)^2} L \frac{B_k}{U_o} \left(\frac{T_o}{1.8}\right)^{\gamma_k} \tag{37}$$

where the necessary conversion factor has been used in order to convert
the density to grm/cm^3 as required. Finally, the dimensionless activation
energy E_k^*, given by Eq. (25) of Part II

$$E_k^* = \frac{E_k}{RT_o}$$

is written in the following form when E_k is given in $cal/gr-mole$, and
T_o in °R:

$$E_k^* \quad \frac{1.8}{1.9857} \frac{E_k}{T_o} \tag{38}$$

C.   Input Data

In addition to the thermodynamic data given in Table I, the follow-
ing input data are required for the solution of the problem. The
various terms are listed in the order in which they appear in the computer
program. This program will be discussed in Section III.

M_e Mach number of the jet at $x = 0$

γ_{jt} Ratio of specific heats for the jet side

T_{T_j} stagnation temperature of the jet (°R)

M_∞ free stream or flight Mach number

M_a Mach number on the air side at $x = 0$

γ_s ratio of specific heats for the air side

T_∞ free stream temperature (°R)

14

p_{T_j} stagnation pressure of the jet (lbs/in^2)

B_L lower (air-side) boundary of the mixing layer

k mesh size in the x-direction

p_{T_s} stagnation pressure of the air stream (lb/in^2)

L reference length, nozzle exit radius (ft)

Pr_t turbulent Prandtl number

Le_t turbulent Lewis number

σ jet spread factor

N number of internal grid points (always an even number)

$(C^i)_a$ concentrations (mass fractions) of species "i" on the air side, $x = 0$

X_i mole fractions of species "i" on the jet side at $x = 0$

$\alpha_o, \alpha_1, \alpha_2, \alpha_3, \alpha_4$ coefficients appearing in the polynomial for H_j [Eq. (9)]

$\beta_{co}, \beta_1, \beta_2, \beta_3, \beta_4$ coefficients appearing in the polynomial for H_s [Eq. (15)]

The above coefficients, as well as H_c and H_a, are obtained from the potential flow solution of the jet[1] and are discussed in Section I. The majority of the data are conditions on the jet or the air stream that must be specified for each particular case. L and k may be selected arbitrarily. A discussion on the value of B_L is given in Section III below.

The values of the turbulent Lewis and Prandtl numbers are not well known. Recent experimental data on recovery factors have indicated a value of $Pr_t \approx 0.86$, and this value may be used for lack of other data. In any case, variations in the Prandtl number are not expected to be large. Data on the turbulent Lewis number is also lacking. The indications are that its value ranges from 1.0 to 1.4. It will be useful to carry out the solution of the present problem for various values of Le_t in this range, in order to determine its effect on the variation of the flow parameters.

The jet spread factor, σ, required in the transformation of the ψ-coordinate is not well known. Experimental values of σ, and its possible variation with Mach number are discussed in the Appendix.

Finally, it should be pointed out that, h, the step size in the ψ-direction, does not appear in the above list. It is computed from B_L and N, as discussed in Section IV of Part II.

III. COMPUTER PROGRAM

The equations derived in Part II, along with the information contained in Sections I and II of this report, were programmed,[*] using the Fortran II system, for calculations on an IBM-704 computer. The program consists of a number of subroutines which are employed as required by the procedure. These subroutines contain numerous descriptive comments and are, in general, self-explanatory. They will be listed here, and discussed briefly, for ease of reference.

Subroutine

INPUT: provides for storage of input data, listed in Section II-C

CONST: used to calculate initial conditions, given in Section I-A, and the reference values of Section II-B

PRELI: executes preliminary operations, such as assigning the initial and boundary conditions

GENV: contains the calculations for functions of x, such as Mach numbers, pressures, pressure gradients, and the variable $F_K(v_K)$ [which contains the reaction term]

BVAL: used for calculating boundary values

FSUBI, FSIP, GIT, and HBI: used to calculate thermodynamic functions $f_i(T)$, $f_i'(T)$, h_{B_i}, and $G_i(T)$ listed in Table I.

MOMEN, SPECI, ENERG: used to calculate all coefficients of momentum, species, and energy equations.

SOLVE: used to solve the above equations simultaneously

INCRE: incrementing subroutine used to obtain the solution of the equations at each successive step in the x-direction

TRANSF: program used for carrying out the transformation of the ψ-coordinate to the physical coordinate y

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[*] The program was prepared by B. Witte and P. Doherty, of the Digital Computer Laboratory, Convair, Astronautics, and was assigned the number 595-420L2.

16

An additional subroutine, denoted as subroutine "MEANS" on the first page of the program, is planned for the future. This subroutine will make it possible to compute the coefficients of the equations at a midpoint of a mesh, rather than at the preceding point, thus improving on the accuracy of the numerical solution.

The number of internal grid points is limited to a maximum of 18, because of the limited memory of the 704 computer. The value of $N = 18$ would require the solution of 144 equations, and the coefficient matrix of these equations would occupy 65 percent of the memory cells, leaving approximately 11000 cells for storage of other quantities, and for the planned subroutine discussed in the preceding paragraph. It is possible by means of an external tape, to increase the capacity of the memory so that values of N larger than 18 may be accomodated. However, the computation time will then be increased from 4 minutes, to approximately 20 minutes, for each step. It may become necessary, at some future date, to use the external tape for at least a few runs in order to be able to evaluate mesh size errors.

The program in its present form allows for only one value of the lower boundary, B_L, to be specified at the start of the solution. The larger the value of B_L, the further downstream can the solution be carried. However, for large values of B_L, the step size in the ψ direction is large, and it becomes difficult to obtain accurate profiles at the initial stages of the mixing layer. It is necessary, then, to start with a small value of B_L, obtain the solution for the first few steps, and, then, restart the program with a larger value, in order to carry the solution further downstream.

To remove this difficulty, it is planned to incorporate into the program a new subroutine which will cause the value of B_L to increase automatically, as the solution progresses. The increase will take place whenever the value of the temperature at the boundary of any given step reaches the usual limit of 99 percent of its asymptotic value.

IV.   TYPICAL CASE AND PRELIMINARY RESULTS

As a typical problem, we will consider the case of a two-dimensional jet of Mach number $M_{jet} = 3.185$ exhausting into an air-stream of Mach number $M_\infty = 5.70$ at an altitude of 150,000 feet. Table II, below, gives the boundary of the jet and the Mach numbers and total pressure at each side of the boundary, as shown in Figure 1a. The coordinates X/r_e and r/r_e are as shown in Figure 1b. The angle ϑ is the angle that the tangent to the boundary makes with the axis of symmetry of the nozzle, and is not used here. The dimensionless coordinate, x (or x^*), used in this work was related to the coordinates of Table II by Eq. (8) as discussed in Section I-B. The following simple relation was found to hold to within ± 1.5 percent:

$$\frac{X}{r_e} = 0.845 \ x$$

The Mach numbers M_j and M_s were expressed as fourth degree polynomials in x. Thus

$$M_j = \alpha_o + \alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3 + \alpha_4 x^4$$

where the values of the coefficients are

$$\alpha_o = 4.86946$$
$$\alpha_1 = .28303$$
$$\alpha_2 = -.64624 \times 10^{-1}$$
$$\alpha_3 = .85049 \times 10^{-2}$$
$$\alpha_4 = -.42125 \times 10^{-3}$$

The stream side Mach number is given by

$$M_s = \beta_{co} + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4$$

with the following values for the coefficients

$$\beta_{co} = 1.96321$$
$$\beta_1 = .29241$$
$$\beta_2 = -.68381 \times 10^{-1}$$
$$\beta_3 = .91005 \times 10^{-2}$$
$$\beta_4 = -.45438 \times 10^{-3}$$

18

TABLE II[*]

DATA OBTAINED FROM THE INVISCID JET FLOW SOLUTION[1] FOR JET
MACH NUMBER M_{jet} = 3.185 AND ALTITUDE 150,000 ft

CHAR	X/r_e	r/r_e	ϑ Degrees	M_j	p_{oj} lb/in^2, ABS	M_s	p_{os} lb/in^2, ABS
J1	0.000	1.000	33.53	4.872	492.0	1.965	3.1
J2	0.090	1.059	33.35	4.896	492.0	1.991	3.1
SO2	0.134	1.088	33.26	4.907	492.0	2.002	3.1
J3	0.179	1.118	33.32	4.928	492.0	2.024	3.1
SU3	0.191	1.126	33.51	4.946	492.0	2.042	3.1
SD3	0.205	1.135	33.30	4.936	492.0	2.032	3.1
SO3	0.270	1.178	33.23	4.955	492.0	2.051	3.1
J4	0.358	1.235	33.17	4.981	492.0	2.079	3.1
J5	0.537	1.352	33.00	5.028	492.0	2.126	3.1
SO7	0.817	1.533	32.807	5.096	492.0	2.196	3.1
SO9	1.096	1.712	32.51	5.147	492.0	2.248	3.1
SD11	1.357	1.877	32.21	5.187	492.0	2.288	3.1
SD16	2.024	2.292	31.67	5.285	492.0	2.387	3.1
J8	2.651	2.674	30.93	5.340	492.0	2.441	3.1
J9	3.515	3.186	30.17	5.412	492.0	2.513	3.1
J10	4.373	3.680	29.65	5.483	492.0	2.584	3.1
J11	5.223	4.160	29.15	5.538	492.0	2.638	3.1
JO12	6.081	4.633	28.66	5.591	492.0	2.691	3.1
SD46	6.529	4.876	28.36	5.614	492.0	2.713	3.1
SU48	6.820	5.032	28.17	5.628	492.0	2.726	3.1

[*]This Table was furnished by Dr. J.M. Bowyer, member of
the Applied Research Group, Convair, Astronautics. It
was computed by the method of characteristics.

19

The error in the above approximations is less than 0.3% of the tabulated values.

In addition to the above coefficients, and the thermodynamic data given in Table I, the following input data were used: (the symbols are defined in Section II-C). $M_c = 4.872$, $\gamma_{jt} = 1.225$, $T_{Tj} = 6300°R$, $M_\infty = 5.700$, $M_a = 1.965$, $\gamma_s = 1.40$, $T_\infty = 505°R$, $p_{Tj} = 492.0$ lbs/in^2, $p_{Ts} = 3.075$ lbs/in^2, $L = 1.91$ ft, $Pr_t = 0.80$, $Le_t = 1.20$, $\sigma = 36.0$, $N = 14$, $B_L = -1.50$ and -3.0, $k = 0.125$.

The concentrations of species at $x = 0$, and at the upper and lower boundaries are

Species*	$(c_i)_a$	X_i
H_2O	0	0.366
H_2	0	0.1420
O_2	0.233	0.0072
CO_2	0	0.1372
CO	0	0.3476
N_2	0.767	0

The value of $B_L = -1.50$ was used to compute the first five steps in the development of the mixing layer ($x = 0.625$). A run was then made with $B_L = -3.0$, and the analysis was carried to $x = 1.25$, i.e., 1-1/4 nozzle exit radii. The results are plotted in Figures 2 through 6, in terms of both the ψ and the y coordinate. The computed reference values are $U_o = 7436.6$ ft/sec and $T_o = 1926.5$ °R. The velocity and concentration profiles, Figures 2, 3, and 6 have the expected trend, and are not affected by the value of B_L. It is noted in Figures 4 and 5 that the temperature profiles exhibit a "bulge" near the x-axis. The peak thus obtained is lower by about 3% for the larger value of B_L (and therefore h). It is believed that this error is the result of the larger mesh size.

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*The values of X_i listed above are based on the results obtained by Neu and Boynton.[2]
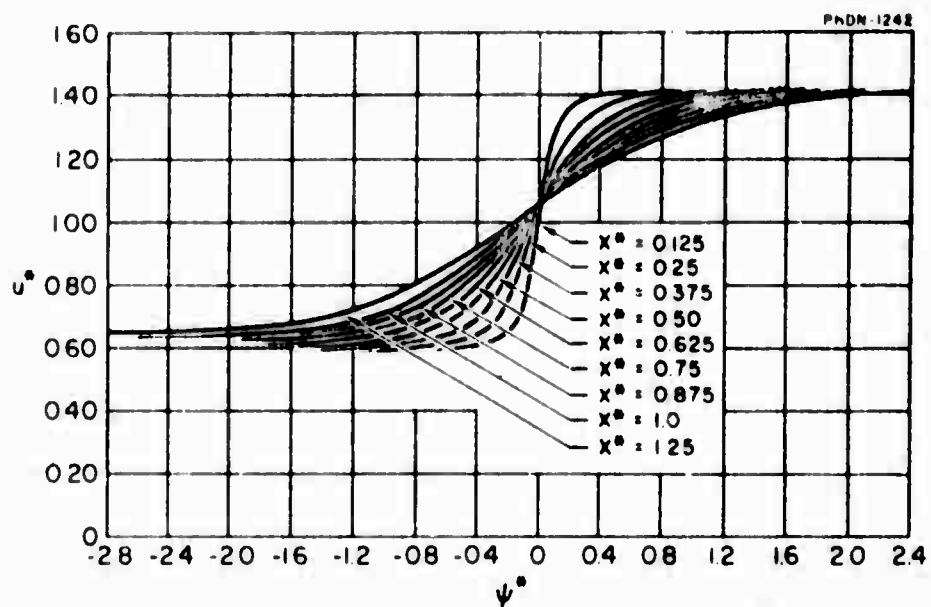
20

FIGURE 2   VELOCITY PROFILES
DURING THE INITIAL STAGES
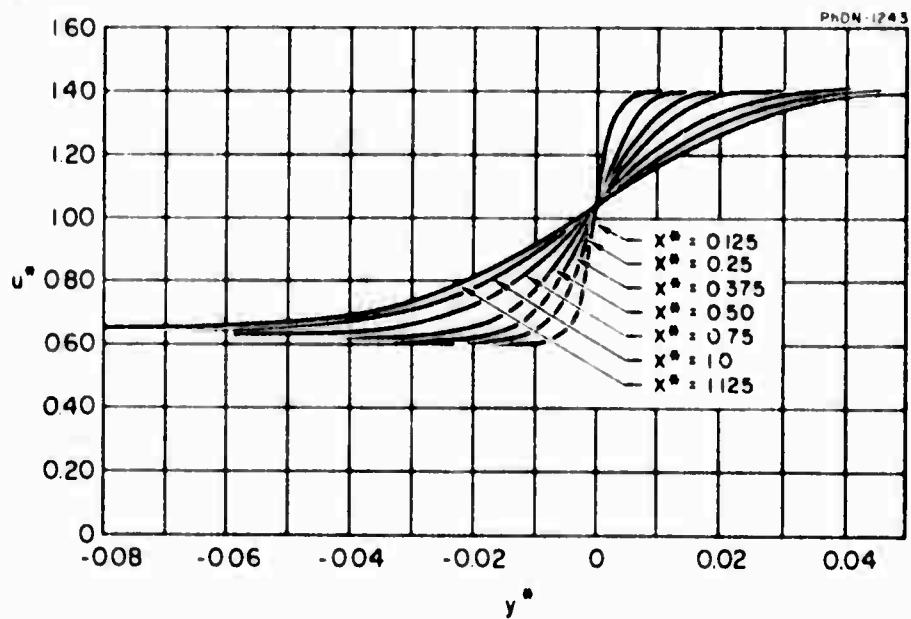OF DEVELOPMENT OF THE MIXING LAYER

FIGURE 3   DIMENSIONLESS VELOCITY VS
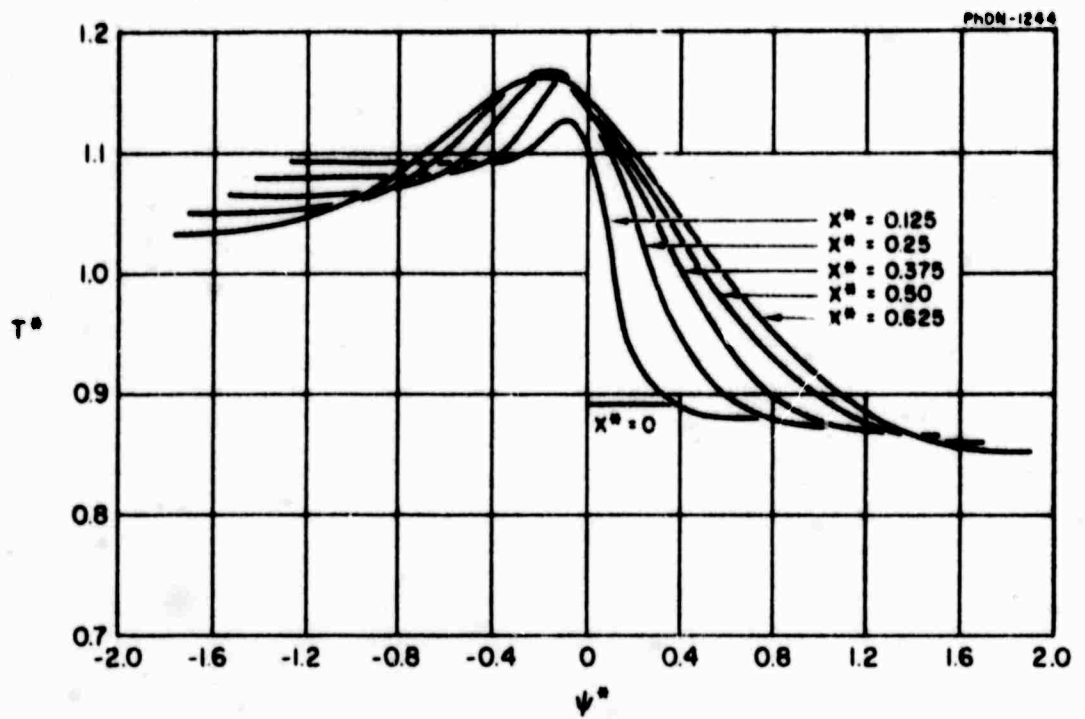THE DIMENSIONLESS COORDINATE y^*
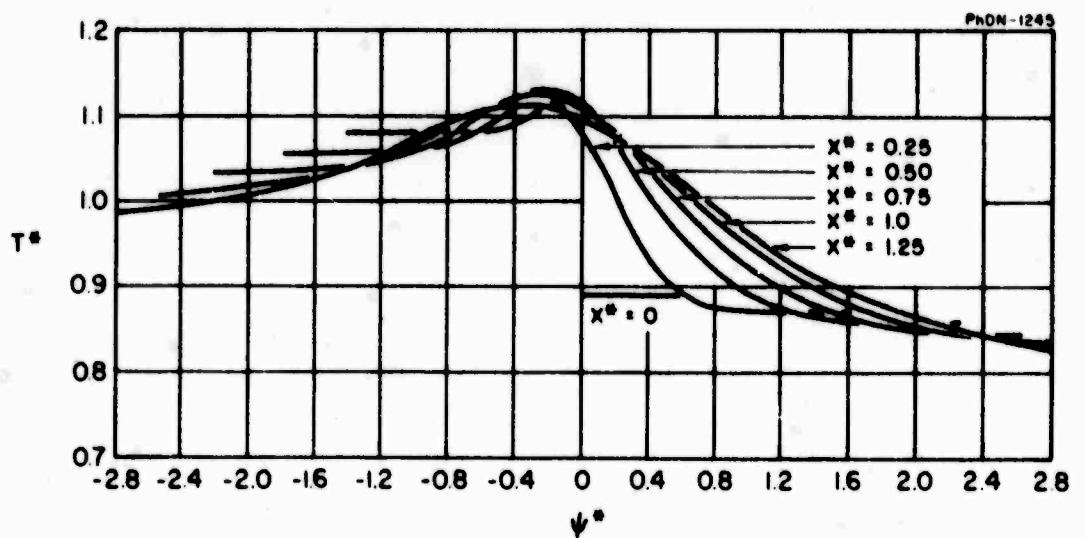
FIGURE 4a   DIMENSIONLESS TEMPERATURE PROFILES

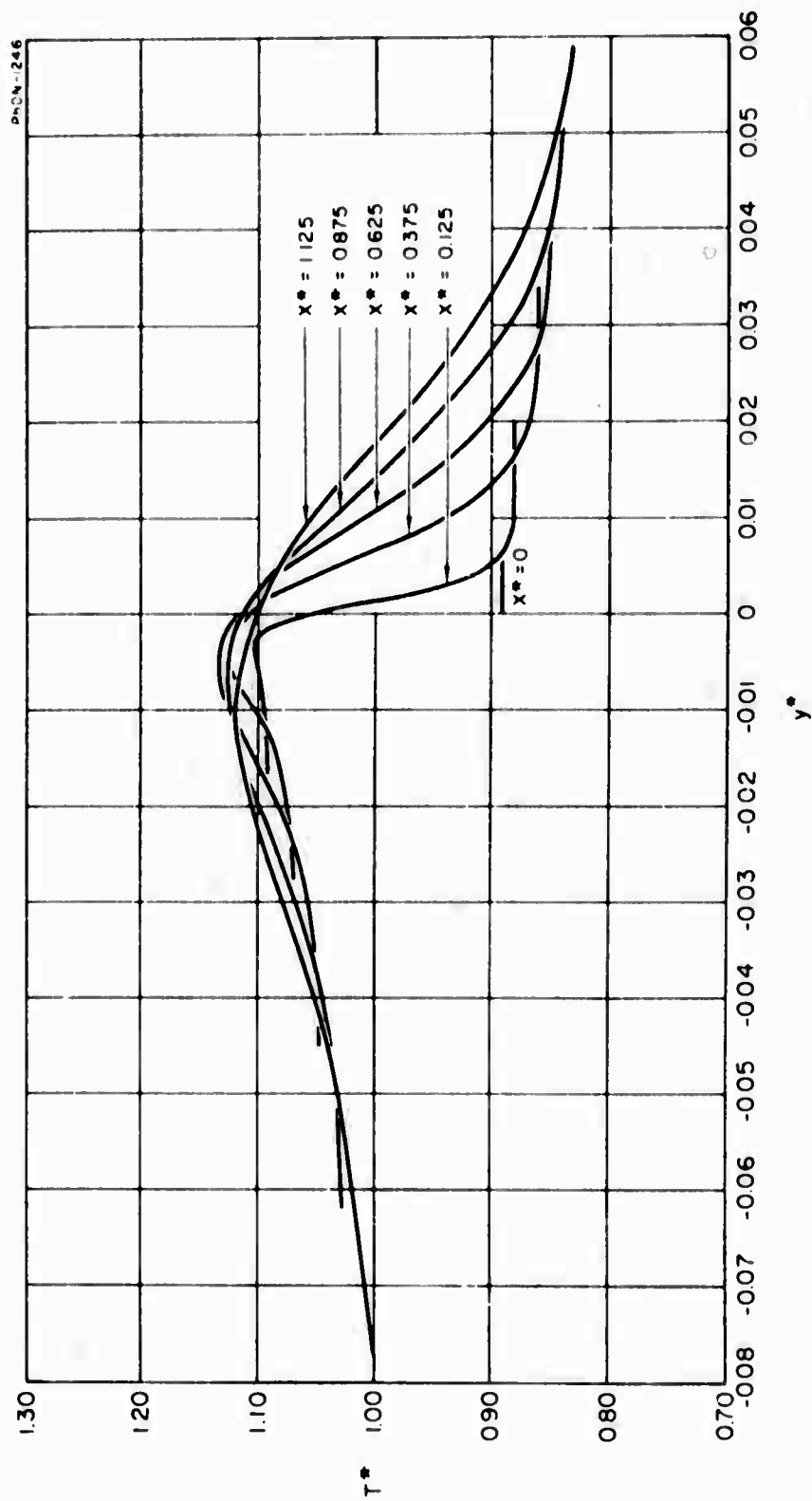

FIGURE 4b   DIMENSIONLESS TEMPERATURE PROFILES

22

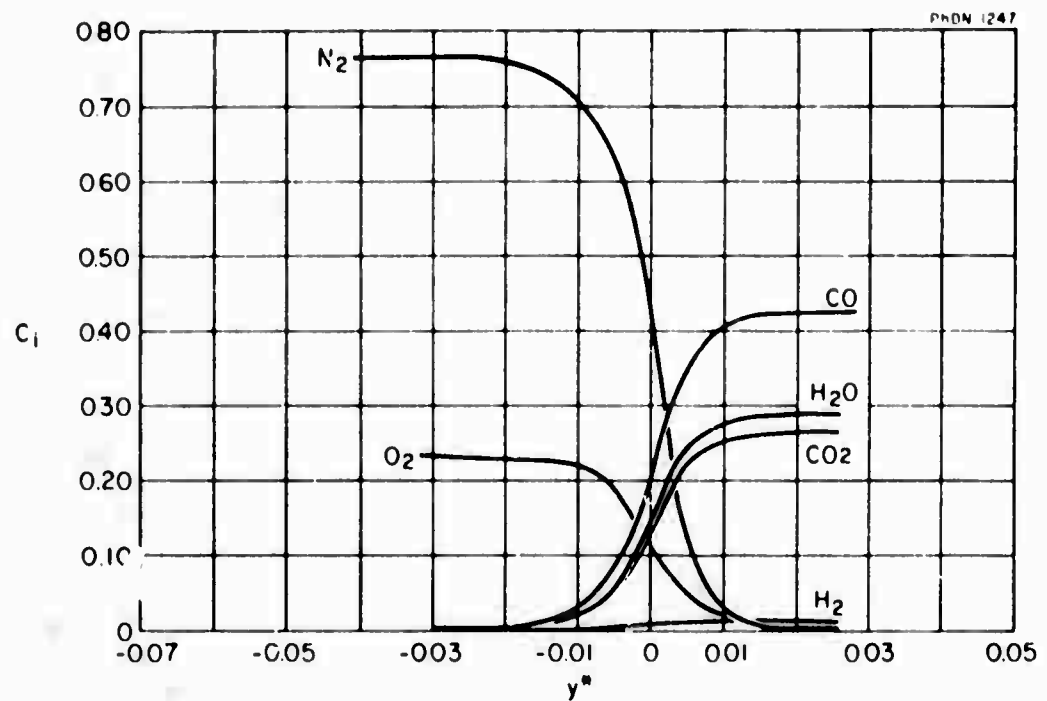FIGURE 5 DIMENSIONLESS TEMPERATURE VS THE DIMENSIONLESS COORDINATE y^*

23

FIGURE 6a CONCENTRATION PROFILES DURING THE INITIAL
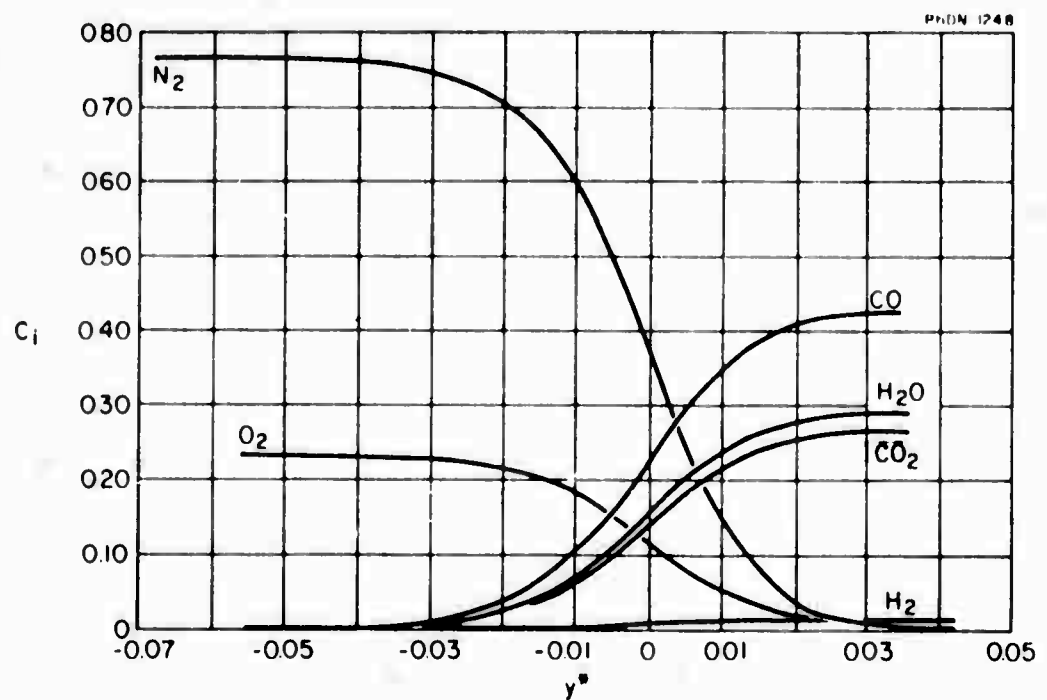STAGES OF DEVELOPMENT OF THE MIXING LAYER, $x^* = 0.25$

FIGURE 6b CONCENTRATION PROFILES DURING THE INITIAL
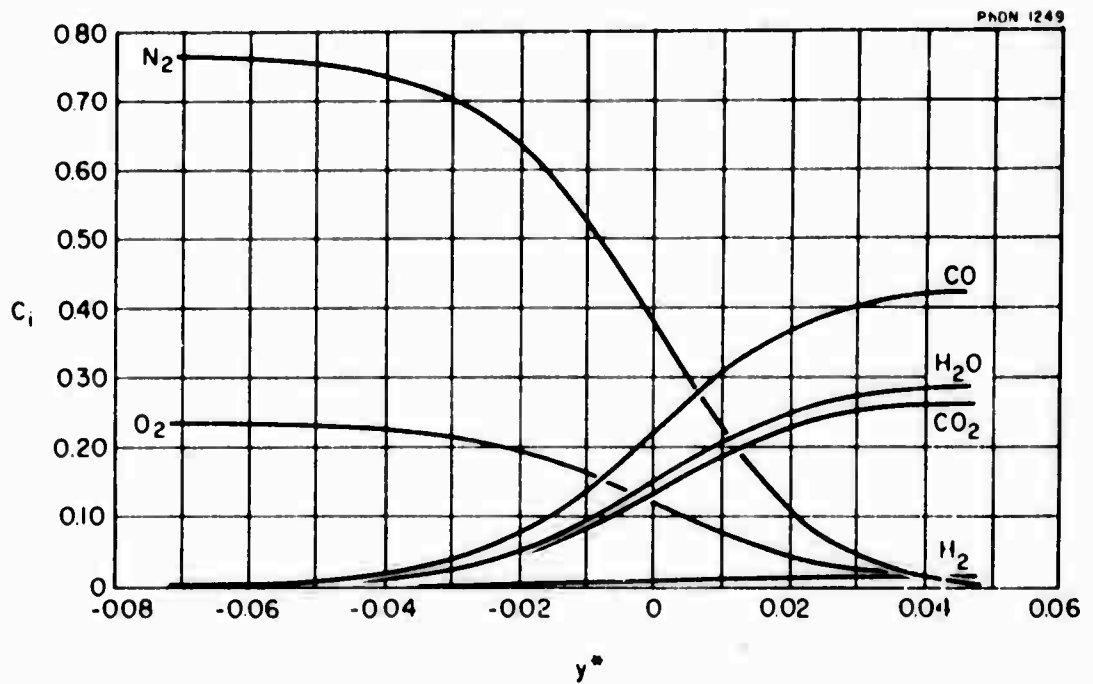STAGES OF DEVELOPMENT OF THE MIXING LAYER, $x^* = 0.50$

FIGURE 6c   CONCENTRATION PROFILES DURING THE INITIAL
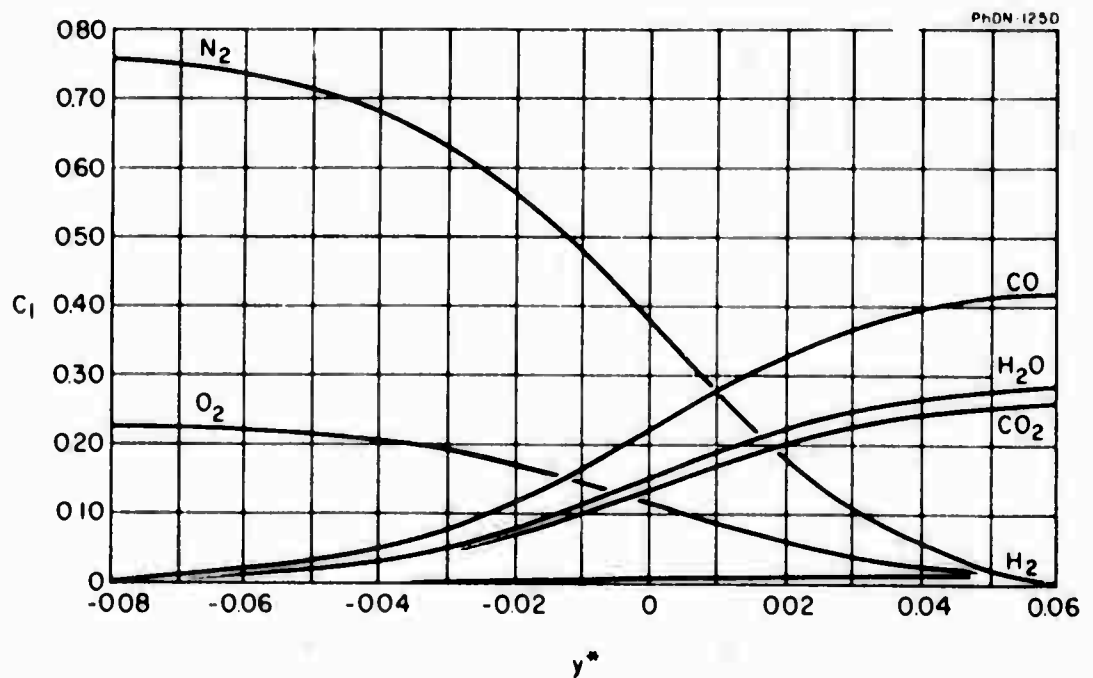STAGES OF DEVELOPMENT OF THE MIXING LAYER, $x^* = 0.75$

FIGURE 6d   CONCENTRATION PROFILES DURING THE INITIAL
STAGES OF DEVELOPMENT OF THE MIXING LAYER, $x^* = 1.125$

In order to determine whether the bulge in the temperature profiles develops into a sharp peak, and also to obtain the thickness of the mixing layer further downstream, the solution was carried to $x = 5.0$ (5 nozzle radii) using $B_L = -12.0$. A plot of the computed thickness is given in Figure 7. To reduce the computation time, the value of k, the step size in the x-direction was doubled. This increase introduced some error in the peak values of the temperature profiles (not reported here). The net increase between the peak value and the asymptotic value at the lower boundary was found to be 14% at $x = 5.0$ as compared to 12.5% at $x = 0.5$. It appears that the cooling of the gases at the boundary, as a result of the expansion, and the low value of the pressure in the mixing layer ($p = 0.17$ lb/in^2 at $x = 5.0$) prevent the bulge in the temperature profile from developing into a sharp peak.

REFERENCES

1. Bowyer, J.M., "Determination of the Envelopes and the Lines of Constant Mach Number for an Axially Symmetric Jet," Convair, Astronautics, Confidential Report No. ZJ-7-054, (March, 1958).

2. Neu, T., and Boynton, F., "Rocket Plume Radiance. Vol. I. - Exit Plane Composition and Temperature," Convair, Astronautics Report No. AZR-014, (December, 1959).
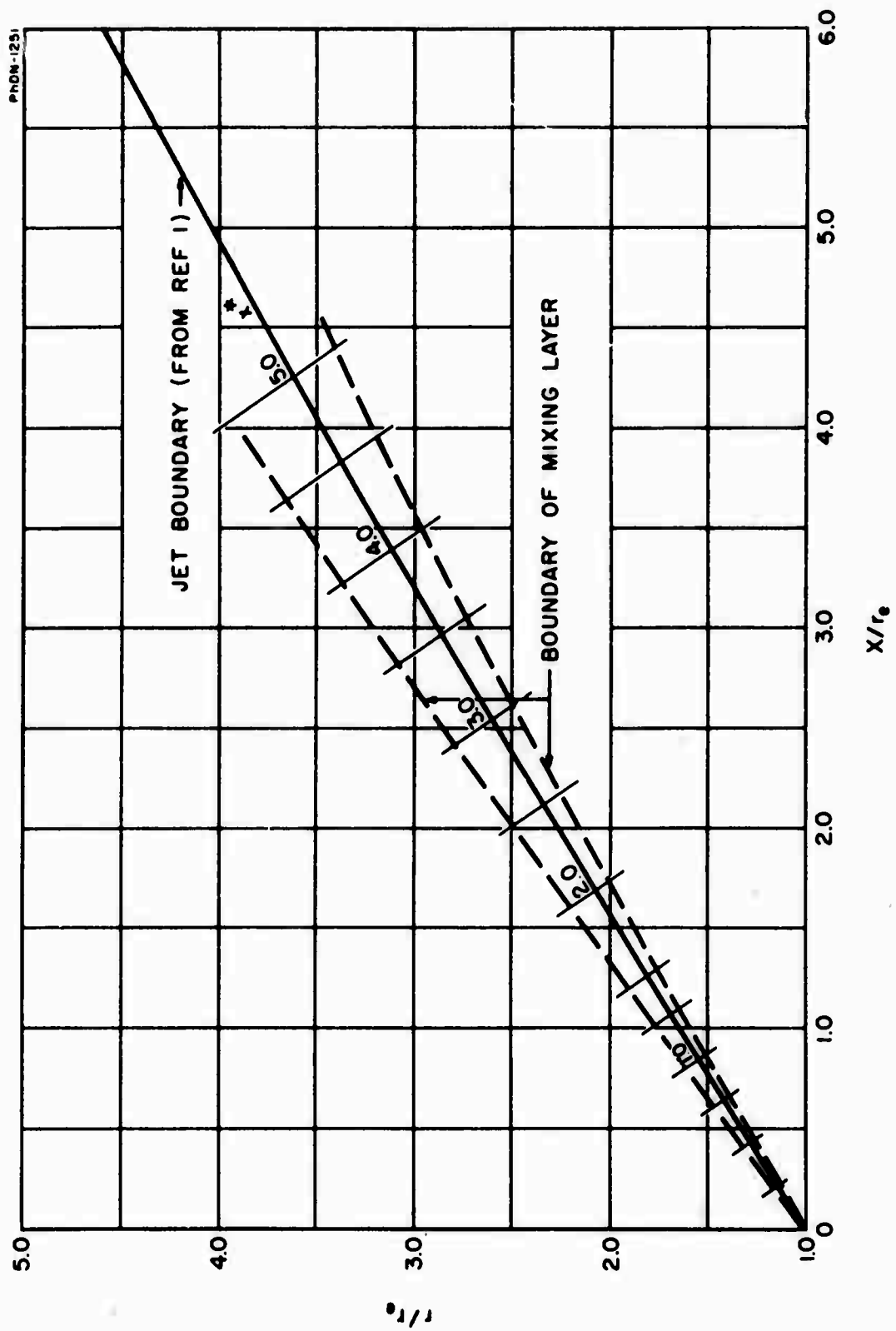
FIGURE 7 COMPUTED THICKNESS OF THE MIXING LAYER

27

NOMENCLATURE

K_{B_k} dimensionless parameter defined by Eq. (37)

L reference length

M Mach number

N number of internal grid points

p pressure (dimensionless when not subscripted, otherwise has the units of lbs/in^2)

p_x dimensionless pressure gradient

r y coordinate of the jet boundary as shown in Figure 1b.

R universal gas constant

R_m gas constant for the mixture

T temperature (dimensionless or in °R as noted)

U velocity at the boundaries (ft/sec)

W_m molecular weight of the mixture

x dimensionless coordinate

X x coordinate of the jet boundary as shown in Figure 1b.

X_i mole fraction of species i

Subscripts

a denotes initial conditions ($x = 0$) for the air-stream side

e initial conditions ($x = 0$) for the jet side

j jet-side conditions for $x > 0$

o reference values

s conditions on the air-stream side for $x > 0$

T_j total or stagnation conditions on the jet side

T_s total conditions on the air-stream side

∞ free stream conditions

28

Greek Symbols

α_o, α_4 coefficients appearing in the polynomial for M_j

β_{co}, β_4 coefficients appearing in the polynomial for M_s

γ_{jt} ratio of specific heats for the jet side

γ_s ratio of specific heats for the air side

σ jet spread factor

APPENDIX

The value of σ is to be obtained from experiments on the rate of spread of supersonic jets. At the present time, the available data are limited to values of $M < 1.60$, and the results of various investigators vary widely, as seen in Figure 8. In this figure, the quantity σ_o refers to the value of σ for an incompressible jet $(M \to 0)$. The value of $\sigma_o = 12$, has been established by numerous experiments. For $M > 2$ values of the ratio σ/σ_o obtained from the experimental data of Anderson and Johns, (Jet Propulsion, Vol. 25, No. 1, 1955) on jets from solid propellant rocket motors have been used, for lack of other data. For $M = 1.40$ and 1.84 the data on hot air jets in this reference is in fair agreement with the results of other investigators. A smooth curve has been drawn through the various points to describe the possible variation of σ/σ_o with M. Obviously this curve is only tentative and should be revised when more information becomes available
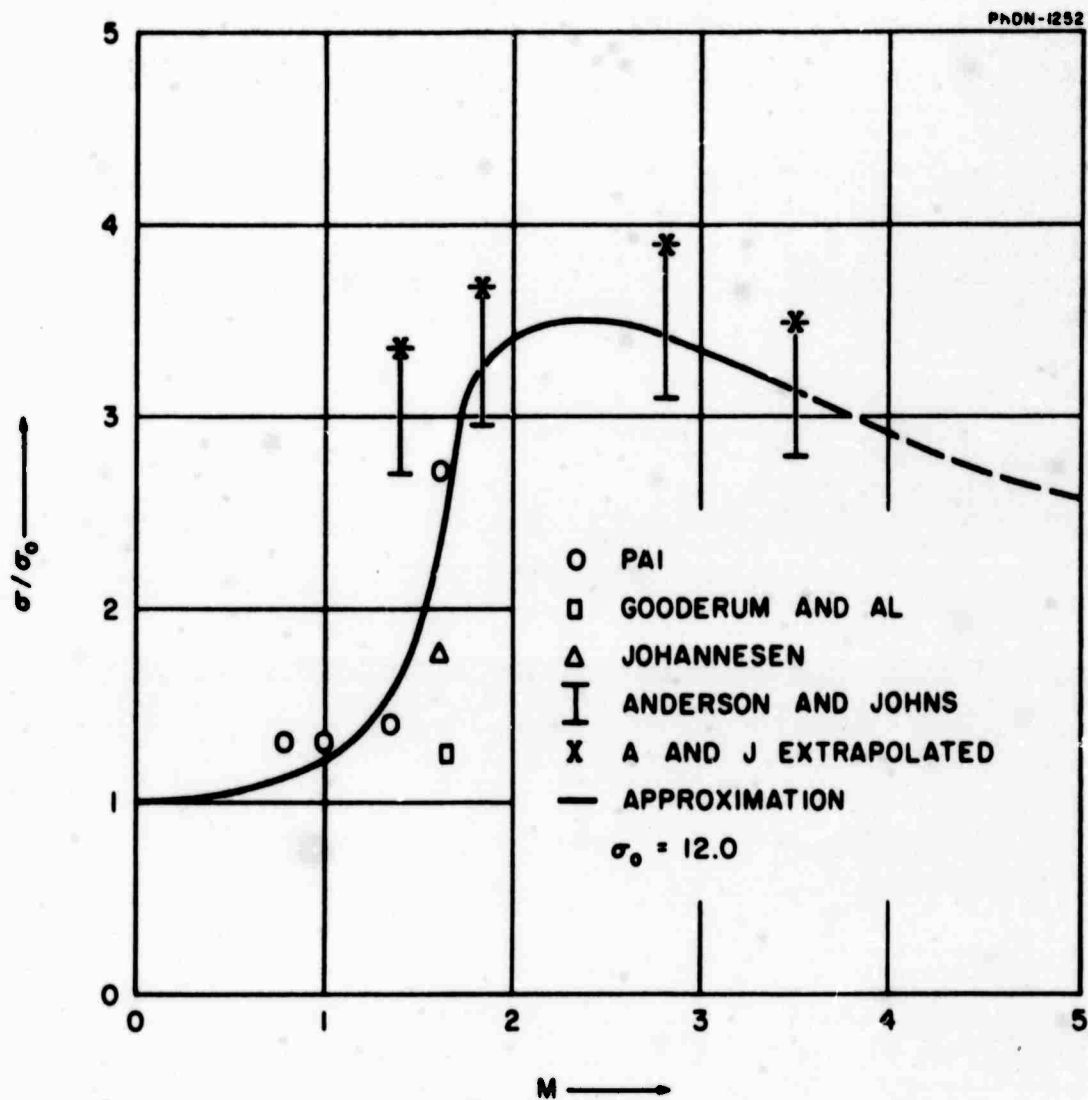
FIGURE 8   EXPERIMENTAL DATA ON THE VALUE OF σ